Development of Liquid Crystal-Based Photovoltaic Technologies

N.R. Armstrong†, B. Kippelen‡, D.F. O'Brien†, S.M. Marder†, J.-L. Brédas†
†Department of Chemistry and ‡Optical Sciences Center
University of Arizona, Tucson, Arizona 85721

ABSTRACT

Under the auspices of NREL/DOE funding we have recently embarked upon a broad program to develop new liquid crystalline-based photovoltaic technologies. Our goal is to combine new self-assembling organic materials that possess charge mobilities of 0.1-1 cm^2/V·s and high charge generation efficiencies, with chemically-modified ITO anodes and new versions of air-stable, low work function Al cathodes, to create a new generation of PV cells. This work builds upon considerable recent work from this group in the development of new organic light emitting diode technologies (OLEDs), development of new self-organizing discotic liquid crystalline materials, new routes for modification of both ITO anodes and cathode materials such as Al, and an expanding theoretical understanding of the critical aspects of exciton dissociation and charge transport in organic thin film materials.

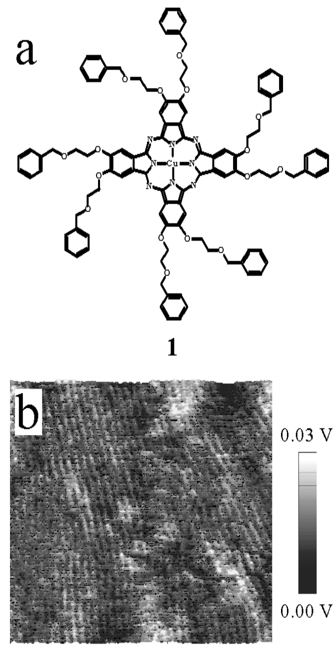


Fig. 1 – Modified phthalocyanine and AFM image of ordered bilayer of rod-like aggregates (Ref).

1. New Discotic Mesophase Materials

Several recent reports have demonstrated that discotic molecular systems can not only form very coherent rod-like assemblies, but that once in these states, the electrical properties of these materials are significantly enhanced.[1,2] Charge mobilities have been observed to be as high as 1cm^2/volt·sec when charge motion is monitored on the 100nm distance scale, and when the average coherence length of these rod-like aggregates is at least of that dimension.

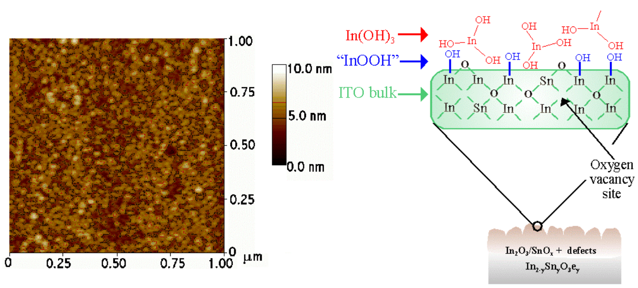
Recent work here at Arizona suggests that phthalocyanines and related macrocycles can be functionalized in such a way as to create coherent aggregates of at least that dimension. Our earliest successes have come from Pcs functionalized with eight benzyl-terminated ethylene oxide side chains (Fig. 1), and horizontally transferred thin films of these molecules have yielded AFM images showing coherence in the Pc rods of at least 100nm.[1,3] Extrapolation of these studies to substrates which will support such columnar structures, with the plane of the Pc parallel to the substrate plane, are underway, as are attempts to create new polymerizable versions of these molecules.[4] Other classes of discotic mesophase materials are in development which incorporate both electron donor and electron acceptor entities in molecular formats which lead to easily processed thin films, and lead to both efficient exciton dissociation and charge transport.

2. Anode/Cathode Interface Characterization/ Modification

Anode and cathode interface composition in PV technologies plays a critical role in determining both efficiencies and lifetimes of these technologies, particularly for organic PV technologies. Recent work at Arizona suggests that interface characterization and modification can have a significant impact on efforts to optimize these technologies.[6,7] Fig. 2 shows an AFM image of a typical ITO surface, along with a schematic view of our current picture of the surface composition of this material.

One of the central technical challenges in using ITO as an anode material in organic solar cells arises as a result of its inherent instability in the presence of even traces of water during its formation, and the difficulty in chemically modifying this interface with hydrophobic groups

Fig. 2 – AFM image of ITO surface, and schematic of its interface composition.



which will also facilitate charge injection processes. Our recent studies, however, suggest that simple chemisorption of redox mediators can be an effective probe of this composition, and can lead to significant enhancements in both PV and OLED device performance.[6]

3. New Directions

We are presently focusing on a) the extrapolation of these results to new discotic mesophase materials, which combine low and high electron affinity molecules in one "super discotic" system; b) new theoretical understandings of exciton dissociation and charge transport in organic thin film materials;[7] and c) new strategies for interface modification of both anode and cathode materials which maximize work function differences and enhance wettability and charge injection rates. Results of this work will be reported at the next NCPV meeting.

4. References

[1] "Highly Ordered Thin Films of Octasubstituted Phthalocyanines," P. Smolenyak, R. Peterson, K. Nebesny, M. Törker, D.F. O'Brien, N.R. Armstrong, J. Amer. Chem. Soc. 121, 8628-8636, (1999).

[2] "The Core-Size Effect on the Mobility of Charge in Discotic Liquid Crystalline Materials," A. M. van de Craats, J. M. Warman, Advanced Materials, 13, 130-133, (2001).

[3] "Transfer of Rod-Like Aggregate Phthalocyanines to Hydrophobized Gold and Silicon Surfaces: Effect of Phenyl-Terminated Surface Modifiers on Thin Film Transfer Efficiency and Molecular Orientation," R.A.P. Zangmeister, D.F. O'Brien, N.R. Armstrong, Langmuir, in-press.

[4] "One-Dimensional Polymers of Octasubstituted Phthalocyanines,"A.S. Drager, R.A.P. Zangmeister, A. Somoygi, N.R. Armstrong, D.F. O'Brien, J. Amer. Chem. Soc., 123, 3595-96, (2001).

[5] "Characterization of Indium-Tin Oxide Interfaces Using X-ray Photoelectron Spectroscopy and Redox Processes of a Chemisorbed Probe Molecule: Effect of Surface Pretreatment Conditions," C.L. Donley, D.R. Dunphy, D. Paine, C. Carter, K.W. Nebesny, P.A. Lee, D. Alloway, N.R. Armstrong, Langmuir, in press.

[6] "Aluminum Composite Cathodes: A New Method for the Fabrication of Efficient and Bright Organic Light Emitting Devices," G.E. Jabbour, S.E. Shaheen, M.M. Morrell, B. Kippelen, and N. Peyghambarian, Optics and Photonics News, 10, 25, (1999).

[7] "Interchain interactions in organic pi-conjugated materials: Impact on electronic structure, optical response, and charge transport," J. Cornil, D. Beljonne, J.P. Calbert, J.-L. Brédas, Advanced Materials, 13, 1053-1067, (2001)